Quantum state discrimination: A geometric approach

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We analyze the problem of finding sets of quantum states that can be deterministically discriminated. From a geometric point of view, this problem is equivalent to that of embedding a simplex of points whose distances are maximal with respect to the Bures distance (or trace distance). We derive upper and lower bounds for the trace distance and for the fidelity between two quantum states, which imply bounds for the Bures distance between the unitary orbits of both states. We thus show that, when analyzing minimal and maximal distances between states of fixed spectra, it is sufficient to consider diagonal states only. Hence when optimal discrimination is considered, given freedom up to unitary orbits, it is sufficient to consider diagonal states. This is illustrated geometrically in terms of Weyl chambers.

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I. INTRODUCTION

In quantum state discrimination, given a set of candidate states, our task is to find out which of the states we have in our possession to the best of our ability [1–3]. A fundamental property of quantum mechanics which adds to the difficulty of this problem is that, on top of possible mixing (that is, statistical sampling over pure states), if two pure states are not orthogonal, they cannot be discriminated perfectly. Two common strategies for discriminating possibly nonorthogonal quantum states are the so-called ambiguous [1] and unambiguous [4] discrimination. In ambiguous discrimination we always end up with an answer, but may sometimes be wrong (and the task is to minimize the probability of being wrong). In unambiguous discrimination we must never be wrong, but (to be consistent with quantum mechanics) may sometimes give a nonanswer, that is we say, we do not know (the task then is to minimize the probability of a nonanswer). Finding an optimal procedure of unambiguous discrimination is particularly interesting if the states analyzed are mixed [5–10].

More generally, the standard approach to the quantum discrimination problem is to begin by considering the discrimination of classical probability distributions and then extend to the quantum setting. This is done via optimizing over measurements. A quantum measurement takes a quantum state to a classical probability distribution over the possible outcomes. For a given measure in the classical setting (quantifying how well we can discriminate probability distributions by some particular figure of merit), the quantum measure is found by taking the classical measure on the probability distributions induced by a measurement, optimized over all possible measurements. Different concepts of the "best" discrimination induce different measures of distinguishability in the space of classical probability distributions. In this way the problem of discriminating quantum states has led to several distance measures associated with the ability to discriminate well (see, e.g., [11–13]). On the other hand, the geometry of state space depends on the distance measure chosen. In this work we would like to consider the geometry induced by these measures, and how the problem of state discrimination can be expressed geometrically.

To be more precise, let $\mathcal{M}_N$ denote the set of mixed quantum states acting on an N-dimensional Hilbert space $\mathcal{H}_N$. It is a convex, compact set of dimensionality N^2-1. Its geometric structure depends on the metric used. The following distances are often used [12,13]:

$$D_{\mathrm{HS}}(\rho_1,\rho_2) := [\mathrm{Tr}(\rho_1-\rho_2)^2]^{1/2}, \tag{1.1}$$

$$D_{\mathrm{tr}}(\rho_1,\rho_2) := \frac{1}{2}\mathrm{Tr}|\rho_1-\rho_2|, \tag{1.2}$$

$$D_{\mathrm{B}}(\rho_1,\rho_2) := [2(1-\mathrm{Tr}|\sqrt{\rho_1}\sqrt{\rho_2}|)]^{1/2}, \tag{1.3}$$

denoting the Hilbert-Schmidt (HS) distance, the trace distance, and the Bures distance respectively. The last quantity is a function of *fidelity* [14],

$$F(\rho_1,\rho_2) := (\mathrm{Tr}|\sqrt{\rho_1}\sqrt{\rho_2}|)^2, \tag{1.4}$$

and the root fidelity $\sqrt{F}$ (which in some papers is also called the fidelity). The Bures and the trace distance are *monotone*,

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and do not grow under the action of an arbitrary quantum operation (completely positive, trace-preserving map), while the Hilbert-Schmidt distance is not monotone. These measures can induce different geometries. For instance, the set $\mathcal{M}_2$ of mixed states of a qubit is equivalent to the standard Bloch ball (the Bloch sphere and its interior) for the trace or HS metric, and to the Uhlmann hemisphere $\frac{1}{2}S^3$ for the Bures distance [15]. For higher N the geometries induced by the HS and the trace distances also differ.

In the following we consider systems of dimension N greater than or equal to 2. We begin our discussion of state discrimination by introducing the diameter of a set of quantum states. The diameter of the set $\mathcal{M}_N$ is given by the maximal possible distance between any of its elements. It is equal to the distance between two orthogonal pure states. This quantity is independent of N, but it does depend on the metric used. A simple calculation shows that the *diameter* of the set of mixed states reads

$$D_{\mathrm{HS}}^{\max} = \sqrt{2}, \quad D_{\mathrm{tr}}^{\max} = 1, \quad D_{\mathrm{B}}^{\max} = \sqrt{2}, \tag{1.5}$$

for HS, trace, and Bures distances, respectively. Any two states separated by $D^{\max}$ are supported on orthogonal subspaces. The reverse implication holds for Bures and trace distances,

$$\mathrm{supp}(\rho_1) \perp \mathrm{supp}(\rho_2) \Leftrightarrow D_{\mathrm{tr}}(\rho_1,\rho_2) = 1 \Leftrightarrow D_{\mathrm{B}}(\rho_1,\rho_2) = \sqrt{2}, \tag{1.6}$$

but is not true for the Hilbert-Schmidt distance for $N>2$. For instance, the HS distance between two diagonal density matrices $\rho_1=\mathrm{diag}(1,0,0)$ and $\rho_2=\mathrm{diag}(0,1/2,1/2)$ is equal to $\sqrt{3/2}<D_{\mathrm{HS}}^{\max}$, although they are supported on orthogonal subspaces. To witness an even more dramatic example, consider the Hilbert space of even dimension N and two diagonal states $\rho_1=\mathrm{diag}(N/2,\ldots,N/2,0,\ldots,0)$ and $\rho_2=\mathrm{diag}(0,\ldots,0,N/2,\ldots,N/2)$. Although they live in orthogonal subspaces, so that their Bures and trace distances are maximal, their HS distance reads $2/\sqrt{N}$ and tends to zero in the limit of large N. This indicates that, when analyzing problems of distinguishability, one cannot therefore rely on the standard Euclidean geometry induced by the Hilbert-Schmidt distance, but should rather use Bures or trace distances.

The trace distance and the Bures distance are, in several respects, good measures for quantifying the ability to discriminate states. In [16] Englert introduced the notion of *distinguishability* between two quantum states and showed that it is equal to the trace distance between them. Hence two states can be deterministically discriminated if they can be perfectly distinguished, so their distinguishability is equal to unity. Fuchs and van de Graaf found a bound between the Bures distance and the trace distance based on the following inequality [12]:

$$1 - \sqrt{F(\rho_1,\rho_2)} \le D_{\mathrm{tr}}(\rho_1,\rho_2) \le \sqrt{1 - F(\rho_1,\rho_2)}. \tag{1.7}$$

This implies that, if the fidelity between both states is equal to zero (so the states are distinguishable and their Bures distance is maximal) their trace distance is equal to unity, and is hence maximal. In fact, the trace distance is a simple function of the probability to successfully discriminate two states in a single-shot measurement (optimized over all allowed quantum measurements) [12]. Similarly, the Bures distance can be seen as the optimized Kullback-Leibler distance between output statistics over all quantum measurements (again, an optimized cost function for discrimination) [11].

In the special case where both density matrices are diagonal and read $\rho_1=\mathrm{diag}(p_1,p_2,\ldots,p_N)$ and $\rho_2=\mathrm{diag}(q_1,q_2,\ldots,q_N)$, the operators commute. Such a case is often called classical since the distances between quantum states reduce then exactly to their classical analogs. The trace distance $D_{\mathrm{tr}}(\rho_1,\rho_1)$ is equal to the L_1 distance between vectors p and q (with a normalization constant 1/2) between both probability vectors. The Bures distance reads $D_{\mathrm{B}}(\rho_1,\rho_2)=\{2[1-B(p,q)]\}^{1/2}$, where

$$B(p,q) := \sum_{i=1}^{N} \sqrt{p_i q_i} \tag{1.8}$$

denotes the *Bhattacharyya* coefficient [17,13]. This quantity is equal to the root fidelity between any two diagonal states, $B(p,q)=\sqrt{F(\rho_1,\rho_2)}$, so its square B^2 is sometimes called the *classical fidelity* between two probability distributions.

In Sec. IV we prove general bounds for the fidelity between two arbitrary quantum states ρ_1 and ρ_2,

$$B^2(p^{\uparrow},q^{\downarrow}) \le F(\rho_1,\rho_2) \le B^2(p^{\uparrow},q^{\uparrow}), \tag{1.9}$$

where the vectors p and q represent the spectra of ρ_1 and ρ_2, while the arrows up (down) indicate that the eigenvalues are put in nondecreasing (nonincreasing) order. These results imply equivalent bounds for the Bures distance,

$$\sqrt{2-2\sqrt{p^{\uparrow}\cdot q^{\uparrow}}} \le D_{\mathrm{B}}(\rho_1,\rho_2) \le \sqrt{2-2\sqrt{p^{\uparrow}\cdot q^{\downarrow}}}. \tag{1.10}$$

Analogous bounds for the trace distance proved in the same section read

$$D_{\mathrm{tr}}(p^{\uparrow},q^{\uparrow}) \le D_{\mathrm{tr}}(\rho_1,\rho_2) \le D_{\mathrm{tr}}(p^{\uparrow},q^{\downarrow}), \tag{1.11}$$

where the symbols $p^{\uparrow}$ and $q^{\downarrow}$ denote here diagonal density matrices with all eigenvalues in nondecreasing (nonincreasing) order.

In this paper we set out to give a geometric interpretation to the problem of state discrimination in terms of the geometries induced by the trace and Bures distances. We are going to use algebraic tools presented by Horn and Johnson [25,26] and Bhatia [27]. We begin in Sec. II by giving a set of conditions on states such that they may be perfectly discriminated. In Sec. III we present some geometrical consequences of these conditions and phrase the problem of state discrimination in terms of the embedding of simplices with respect to different distance functions. In Sec. IV we investigate the distance between states under unitary orbits and its geometric interpretation, and prove the above bounds. We finish in Sec. V with conclusions. More technical proofs needed for Sec. IV are left to the appendixes.

II. PERFECT DISCRIMINATION OF STATES

We begin by looking at some conditions on the set of states that can be perfectly discriminated. By perfect discrimination, we mean that by choosing an appropriate measurement we can say with absolute certainty which state we have out of the set, unlike the unambiguous and ambiguous discrimination discussed in the introduction. Our condition will follow from simple analysis of the measurements [in terms of the associated positive operator valued measure (POVM)], and give general conditions which, in the next section, will be used to give some geometrical consequences of the problem.

Theorem 1. Two states ρ_1 and ρ_2 can be deterministically discriminated if and only if their supports do not overlap.

Proof. Any perfect state discrimination strategy for two states ρ_1 and ρ_2 can be written as a three-element POVM $\{A_1, A_2, A_?\}$, where the outcomes correspond to concluding it is the state ρ_1, ρ_2, and allowing for inconclusive outcomes, respectively.

Note that, although in general we can have far more possible outcomes than three, this formalism does include all possible discrimination strategies—this is because we can always group the outcomes corresponding to state ρ_1 to give A_1, and those to state ρ_2 to give A_2, and the remaining elements we group to give $A_?$. The probability of success of the strategy can always be written in terms of such POVMs; thus we can restrict ourselves to only these three-element POVMs for perfect discrimination.

The conditions on the POVM for deterministic state discrimination are

$$\mathrm{Tr}(A_1\rho_1) = 1, \tag{2.1}$$

$$\mathrm{Tr}(A_2\rho_2) = 1, \tag{2.2}$$

$$A_1 + A_2 + A_? = \mathbf{1}, \tag{2.3}$$

$$\mathbf{1} \geq A_i \geq 0 \tag{2.4}$$

(this is the same logic as in [18], only without the separability condition). The first two are necessary for perfect state discrimination since the probability of state ρ returning outcome A_i is given by $\mathrm{Tr}(A_i\rho)$. As a side note, these conditions can easily be extended to consider imperfect discrimination, by allowing different values for the probabilities on the right-hand side of conditions (2.1) and (2.2). Any optimizing strategy would then optimize over the POVM according to the given cost function (for example, unambigious or ambiguous discrimination, or the distance functions mentioned in the Introduction). For now we consider only perfect discrimination. Conditions (2.3) and (2.4) are just the conditions for $\{A_i\}$ to be a POVM.

Conditions (2.1) and (2.2) imply that the elements A_1 and A_2 include projections onto the support of ρ_1 and ρ_2, respectively. To see this, rewrite (2.1) in the eigenbasis of $\rho_1 = \Sigma_i \lambda_i |i\rangle\langle i|$ [we extend this basis to the full space for writing A_1 in (2.6)]

$$\mathrm{Tr}(A_1\rho_1) = \sum_i \lambda_i \langle i|A_1|i\rangle = \sum_i \lambda_i q_i = 1, \tag{2.5}$$

where $q_i := \langle i|A_1|i\rangle$ is a probability, hence $\Sigma_i \lambda_i q_i \leq 1$ and equality is obtained only when $q_i = 1$ for all i such that $\lambda_i \neq 0$. If we also demand conditions (2.3) and (2.4) the most general A_k can be written

$$A_k = P_k + \sum_{i,j \notin \mathrm{Supp}(\rho_1), \mathrm{Supp}(\rho_2)} \alpha_{i,j} |i\rangle\langle j|, \tag{2.6}$$

where $P_k = \Sigma_{i \in \mathrm{Supp}(\rho_k)} |i\rangle\langle i|$ is the projector onto the support of state ρ_k. The projectors onto the support of a state ρ, with eigendecomposition $\rho = \Sigma_j \alpha_j |j\rangle\langle j|$ is given by $P = \Sigma_j |j\rangle\langle j|$. From here, condition (2.3) clearly says

$$\begin{aligned} & P_1 + P_2 \leq \mathbf{1} \\ & \Rightarrow \mathrm{Tr}(P_1 P_2) = 0 \\ & \Rightarrow \mathrm{Tr}(\rho_1 \rho_2) = 0 \\ & \Rightarrow \mathrm{Tr}|\rho_1 - \rho_2|/2 = 1. \end{aligned} \tag{2.7}$$

Hence the supports have zero overlap. ■

The theorem is easily extended to sets of states $\{\rho_i\}_{i=1}^M$.

Theorem 2. The states $\{\rho_i\}_{i=1}^M$ can be deterministically discriminated if and only if their supports do not overlap.

This directly leads to the following proposition.

Proposition 1. Consider K states acting on the N-dimensional Hilbert space, which can be discriminated deterministically. Then

$$\sum_{i=1}^{K} \mathrm{rank}(\rho_i) \leq N. \tag{2.8}$$

This proposition is clear from the theorem, but also can be derived from the result in [18]. This is done by taking the zero-entanglement case of the main result presented there. Specifically, the left-hand side of the inequality in [[18], Eq. (8)] for zero entanglement, along with [[18], Eq. (1)] give exactly (2.8).

III. SOME GEOMETRICAL CONSEQUENCES

We now look at what the above results have to say in terms of the geometric interpretation of the problem of state discrimination. Due to property (1.6), the above theorem can also be formulated as the condition that the trace (or Bures) distance between states is maximal. This fact has an immediate geometric implication. Let us start to work with the trace distance and denote by $\Delta_k \subset \mathbb{R}^k$ a maximal regular *k-simplex* defined by $k+1$ points with mutual trace distance between points equal to $D_{\mathrm{tr}}^{\max} = 1$. As a consequence of Proposition 1 we obtain the following result.

Proposition 2. Let R be an arbitrary convex subset of $\mathcal{M}_N$. Assume that there exists a maximal simplex $\Delta_k \subset R$ and assume that R does not contain Δ_{k+1}. Then the maximal number of states of R which can be discriminated deterministically is equal to $k+1$.

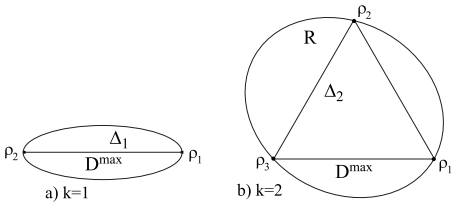

FIG. 1. Set R of positive operators with $k+1=$(a) 2 and (b) 3 distinguishable states $\rho_1,\ldots,\rho_{k+1}$ which form a k-dimensional simplex Δ_k of maximal side length $D^{\max}$, with respect to the Bures (or the trace) metric.

An analogy of Proposition 2 may be formulated for the geometry induced by the Bures distance.

Thus the problem of finding the maximal number of distinguishable states on a certain set is equivalent to the problem of embedding inside it a regular simplex of maximal dimensionality with the diameter given by $D^{\max}$ (see Fig. 1).

At this point it is worth mentioning a different quantum problem of finding "symmetric, informationally complete positive operational valued measures" (SIC POVMs) [19]. This has a similar geometric interpretation of inscribing inside the set $\mathcal{M}_N$ of mixed states an (N^2-1)-dimensional simplex spanned by N^2 pure states $|\phi_j\rangle$, the overlap of which is constant, $F=|\langle\phi_i|\phi_j\rangle|^2=1/(N+1)$ for any $i\neq j$. Therefore, in this case, the side of the simplex with respect to the Bures distance reads $D_{\mathrm{B}}^{\mathrm{SIC}}=\sqrt{2(1-\sqrt{F})}=\sqrt{2-2/\sqrt{N+1}}$, and for a finite dimension N, this is smaller than $D_{\mathrm{B}}^{\max}=\sqrt{2}$.

So in the distinguishability problem we wish to embed into the set $\mathcal{M}_N$ of mixed states a simplex of the maximal side length $D_{\mathrm{B}}^{\max}$ with dimensionality not larger than N, while in the SIC POVM problem we try to inscribe inside the same set a higher-dimensional simplex of a smaller side length $D_{\mathrm{B}}^{\mathrm{SIC}}$.

IV. DISTANCES BETWEEN UNITARY ORBITS

In this section we shall be concerned with the distances between orbits generated from quantum states by unitaries. That is, given two states ρ_1 and ρ_2 with fixed spectra, we wish to know how "distant" or how "close" we can make these states by unitary action. We will find that for the Bures and trace distances the closest and the farthest that can be achieved are given when both states are diagonal in the same basis. This has a geometric interpretation in terms of the Weyl chambers as will be discussed.

This problem can be interesting in many areas of quantum information. Operationally the problem of finding the best unitary separation of two density matrices may be interesting if we are restricted to certain spectra or mixedness. For example, in coding for noisy channels, if we know that the output of some channel will imply a certain mixedness (or even specific spectra), we naturally want to choose to encode on states that are least affected by this. If we are encoding classical information, this will be those states that remain most distinguishable afterward. A simple example of such a channel would be one that probabilistically adds white noise. Freedom of the input state would correspond to unitary freedom of the outputs states which we wish to optimize over, hence considering the optimum over unitary orbits of the output mixed states is equal to finding the optimum encoding. We will see that, in such cases, when only the spectra are restricted, the worst and best cases are given by taking them diagonal in the same basis.

Consider first two classical, N-point, normalized probability distributions $p=(p_1,\ldots,p_N)$ and $q=(q_1,\ldots,q_N)$ such that $p_i,q_i\geq 0$ and $\Sigma_i p_i=\Sigma_i q_i=1$. As earlier, let $p^{\downarrow}$ denote the vector ordered in decreasing order, $p_i^{\downarrow}\geq p_{i+1}^{\downarrow}$, while let $p_i^{\uparrow}$ represent components of the probability vector in increasing order, $p_i^{\uparrow}\leq p_{i+1}^{\uparrow}$.

Any quantum state ρ_1 generates an orbit of unitarily equivalent states, $U\rho_1U^{\dagger}$. Two states ρ_1 and $U\rho_1U^{\dagger}$ are sometimes called *geometrically uniform* and they have been recently considered in the context of unambiguous discrimination [6,7,10].

We are going to discuss another problem of distinguishing states from two orbits. Consider two diagonal quantum states $\rho_1=\mathrm{diag}(p)$ and $\rho_2=\mathrm{diag}(q)$ from which we construct two orbits of unitarily equivalent states. We shall analyze the minimal and maximal distance D_x between the orbits,

$$M(\rho_1,\rho_2):=\max_{U,V} D_x(U\rho_1U^{\dagger},V\rho_2V^{\dagger})=\max_{W} D_x(\rho_1,W\rho_2W^{\dagger}), \tag{4.1}$$

$$m(\rho_1,\rho_2):=\min_{U,V} D_x(U\rho_1U^{\dagger},V\rho_2V^{\dagger})=\min_{W} D_x(\rho_1,W\rho_2W^{\dagger}), \tag{4.2}$$

since performing maximization over two unitary matrices U and V is equivalent to finding a single unitary matrix $W=U^{\dagger}V$. Here D_x stands for one of the monotone distances D_{B} or D_{tr}.

We conjecture that extrema for these distances are obtained for diagonal matrices. Then the extremization has to be performed only over the group P of permutation matrices, which change the order of the spectra,

$$M(\rho_1,\rho_2)=\max_{P} D_x(p,q)=D_x(p^{\downarrow},q^{\uparrow})=D_x(p^{\uparrow},q^{\downarrow}), \tag{4.3}$$

$$m(\rho_1,\rho_2)=\min_{P} D_x(p,q)=D_x(p^{\downarrow},q^{\downarrow})=D_x(p^{\uparrow},q^{\uparrow}). \tag{4.4}$$

The minimum is then achieved for the same order of components in both vectors, while the maximum occurs for opposite ordering, so by using the above formula one can evaluate analytically the extremal distances for both distances in consideration. A similar statement for the nonmonotone Hilbert-Schmidt distance (1.1) was already proved in [20], encouraging this conjecture, and it will give some intuitively sensible and pleasing geometric interpretations in terms of Weyl chambers as will be discussed. We will proceed to prove the validity in the following.

Let us first show that this conjecture holds for the Bures distance.

Theorem 3. The maximum and minimum Bures distances between the unitary orbits of two states are given by diagonal states with

$$M(\rho_1,\rho_2)=\max_P D_{\mathrm{B}}(p,q)=D_{\mathrm{B}}(p^{\downarrow},q^{\uparrow})=D_{\mathrm{B}}(p^{\uparrow},q^{\downarrow}) \tag{4.5}$$

and

$$m(\rho_1,\rho_2)=\min_P D_{\mathrm{B}}(p,q)=D_{\mathrm{B}}(p^{\downarrow},q^{\downarrow})=D_{\mathrm{B}}(p^{\uparrow},q^{\uparrow}). \tag{4.6}$$

Proof. (a) We start by providing an upper bound for the Bures distance (1.3). Let us start with the inequality

$$\sqrt{p^{\uparrow}}\cdot\sqrt{q^{\uparrow}}\geq \mathrm{Tr}\sqrt{\rho_1}\sqrt{\rho_2}\geq \sqrt{p^{\uparrow}}\cdot\sqrt{q^{\downarrow}}, \tag{4.7}$$

which is a particular case of (A1) from Lemma 3 proved in Appendix A. Since $\mathrm{Tr}|\sqrt{\rho_1}\sqrt{\rho_2}|\geq \mathrm{Tr}\sqrt{\rho_1}\sqrt{\rho_2}$, we immediately infer that the root fidelity is bounded from below by the Bhattacharyya coefficient between the spectra put in opposite order,

$$\sqrt{F(\rho_1,\rho_2)}=\mathrm{Tr}|\sqrt{\rho_1}\sqrt{\rho_2}|\geq \mathrm{Tr}\sqrt{\rho_1}\sqrt{\rho_2}\geq \sqrt{p^{\uparrow}}\cdot\sqrt{q^{\downarrow}}=B(p^{\uparrow}q^{\downarrow}). \tag{4.8}$$

This implies an upper bound for the Bures distance which is clearly achievable, $M(\rho_1,\rho_2)=D_B(p^{\uparrow},q^{\downarrow})$. ■

In this way we obtain a general upper bound (4.5) for the Bures distance between any two density operators with spectra p and q,

$$D_{\mathrm{B}}(\rho_1,\rho_2)\leq D_{\mathrm{B}}(p^{\uparrow},q^{\downarrow})=[2(1-\sqrt{p^{\uparrow}}\cdot\sqrt{q^{\downarrow}})]^{1/2}. \tag{4.9}$$

(b) Next we provide a lower bound for the Bures distance (1.3). To prove the case for minimization our task is to show

$$\sqrt{p^{\uparrow}}\cdot\sqrt{q^{\uparrow}}\geq \mathrm{Tr}|\sqrt{\rho_1}\sqrt{\rho_2}|, \tag{4.10}$$

or equivalently to get an upper bound for the root fidelity $\sqrt{F(\rho_1,\rho_2)}$.

First we note that for any operator A we have [12,21,26]

$$\max_U|\mathrm{Tr}\,UA|=\mathrm{Tr}\sqrt{AA^{\dagger}}\equiv \mathrm{Tr}|A|\equiv\|A\|_1, \tag{4.11}$$

where the maximum is taken over all unitaries U. We will also use the von Neumann inequality [22], which concerns the absolute value of the trace of a product of two matrices and their singular values.

Lemma 1 (von Neumann inequality). Let $\sigma_1(A),\ldots,\sigma_n(A)$ and $\sigma_1(B),\ldots,\sigma_n(B)$ denote singular values of the matrices A and B arranged in nonincreasing order. For any matrices A and B the following inequality holds:

$$|\mathrm{Tr}\,AB|\leq\sum_{i=1}^{n}\sigma_i(A)\sigma_i(B). \tag{4.12}$$

For a recent exposition see [23] and [24].

Without losing generality we can assume that ρ_1 is diagonal, $\rho_1=\mathrm{diag}(p)$ and $\rho_2=V\,\mathrm{diag}(q)V^{\dagger}$. Then

$$\max_V\sqrt{F}(\rho_1,\rho_2)=\max_V\mathrm{Tr}|\sqrt{\rho_1}\sqrt{\rho_2}|=\max_V\mathrm{Tr}|\sqrt{p}V\sqrt{q}V^{\dagger}|. \tag{4.13}$$

Using (4.11) and the cyclic property of the trace we get

$$\max_V\sqrt{F}(\rho_1,\rho_2)=\max_{V,U}|\mathrm{Tr}\,U\sqrt{p}V\sqrt{q}V^{\dagger}|=\max_{V,U}|\mathrm{Tr}\sqrt{p}V\sqrt{q}V^{\dagger}U| \tag{4.14}$$

$$=\max_{V,W}|\mathrm{Tr}\sqrt{p}V\sqrt{q}W| \tag{4.15}$$

where $W=V^{\dagger}U$ is unitary. Since the vectors $\sqrt{p}$ and $\sqrt{q}$ contain singular values of matrices $\sqrt{p}V$ and $\sqrt{q}W$, respectively, it follows from (4.12) that

$$|\mathrm{Tr}\sqrt{p}V\sqrt{q}W|\leq\sum_{i=1}^{n}\sigma_i^{\uparrow}(\sqrt{p}V)\sigma_i^{\uparrow}(\sqrt{q}W). \tag{4.16}$$

Thus we get the bound for the maximal root fidelity of the unitary orbit,

$$\max_V\sqrt{F}(\rho_1,\rho_2)\leq\sum_{i=1}^{n}\sigma_i^{\uparrow}(\sqrt{p}V)\sigma_i^{\uparrow}(\sqrt{q}W) \tag{4.17}$$

$$=\sqrt{p^{\uparrow}}\cdot\sqrt{q^{\uparrow}}. \tag{4.18}$$

This result implies the desired upper bound for the root fidelity,

$$\sqrt{F}(\rho_1,\rho_2)\leq\sqrt{p^{\uparrow}}\cdot\sqrt{q^{\uparrow}}, \tag{4.19}$$

which finishes the proof of the lower bound (4.6). Squaring the relations (4.8) and (4.19) we establish the inequalities (1.9) and (1.10). ■

Now we are going to formulate and prove an analogous conjecture for the trace distance.

Theorem 4. The maximum and minimum trace distances between the unitary orbits of two states are given by diagonal states with

$$M(\rho_1,\rho_2)=\max_P D_{\mathrm{tr}}(p,q)=D_{\mathrm{tr}}(p^{\downarrow},q^{\uparrow})=D_{\mathrm{tr}}(p^{\uparrow},q^{\downarrow}) \tag{4.20}$$

and

$$m(\rho_1,\rho_2)=\min_P D_{\mathrm{tr}}(p,q)=D_{\mathrm{tr}}(p^{\downarrow},q^{\downarrow})=D_{\mathrm{tr}}(p^{\uparrow},q^{\uparrow}). \tag{4.21}$$

Proof. The above theorem can be expressed in term of singular values as

$$\sum_{i=1}^{n}|\sigma_i(\rho_1)-\sigma_i(\rho_2)|\leq\sum_{i=1}^{n}\sigma_i(\rho_1-\rho_2)\leq\sum_{i=1}^{n}|\sigma_i(\rho_1)-\sigma_{n+1-i}(\rho_2)|. \tag{4.22}$$

Here $\sigma_i(\rho_1)$ and $\sigma_i(\rho_2)$ denote decreasingly ordered singular values of both operators.

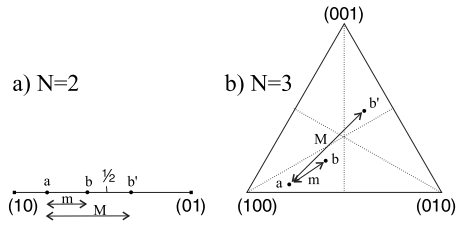

FIG. 2. Simplex of eigenvalues for $N=$(a) 2 and (b) 3, split into $2!=2$ (left and right) and $3!=6$ (indicated by dotted lines) Weyl chambers, respectively. The minimal distance m between the orbits of unitarily similar states stemming from two quantum states is equal to the distance between the corresponding spectra a and b belonging to the same Weyl chamber shown for $N=$(a) 2 and (b) 3. The maximal distance M is achieved for points a and b' belonging to the opposite Weyl chambers.

The lower bound follows from the special case ($k=n$) of the following lemma from [26].

Lemma 2. Let $A,B\in M_n$, and suppose $A,B,A-B$ have decreasingly ordered singular values $\sigma_1(A)\geq\cdots\geq\sigma_n(A)$, $\sigma_1(B)\geq\cdots\geq\sigma_n(B)$, $\sigma_1(A-B)\geq\cdots\geq\sigma_n(A-B)$. Define $s_i(A,B)\equiv|\sigma_i(A)-\sigma_i(B)|$ and let $s_{[1]}(A,B)\geq\cdots\geq s_{[n]}(A,B)$ denote a decreasingly ordered rearrangement of the values $s_i(A,B)$. Then

$$\sum_{i=1}^{k} s_{[i]}(A,B)\leq\sum_{i=1}^{k}\sigma_i(A-B)\quad\text{for } k=1,2,\ldots,n. \tag{4.23}$$

The upper bound in (4.22) follows from Lemma 5 in Appendix B if A and B are positive semidefinite. Since any density matrix ρ is positive, its eigenvalues and singular values are equal. Making use of the definition (1.2) we obtain therefore the required bounds for the trace distance

$$2D_{\mathrm{tr}}(p^{\downarrow},q^{\downarrow})\leq\mathrm{Tr}|\rho_1-\rho_2|\leq 2D_{\mathrm{tr}}(p^{\downarrow},q^{\uparrow}) \tag{4.24}$$

equivalent to Eq. (1.11). ■

We now consider what this means geometrically, and we will do this in terms of the so-called Weyl chamber. A Weyl chamber is a simplex of ordered eigenvalues, i.e., it is formed of part of the simplex of eigenvalues in which all of the eigenvalues follow a prescribed order. Since in a set of N elements there exist $N!$ permutations, the regular simplex of eigenvalues of a density matrix of size N contains $N!$ Weyl chambers (see, e.g., [13]). Any unitary orbit is generated from an ordered spectrum of the density matrix, which corresponds to a point inside a single Weyl chamber. Thus the minimal distance between a diagonal state ρ_1 and a unitary orbit stemming from ρ_2 is obtained at the point in which the orbit intersects the Weyl chamber distinguished by ρ_1. This implies that the mimimum is achieved if both matrices are diagonal and both spectra follow the same order. On the other hand the maximum is achieved for a diagonal ρ_2 with permuted eigenvalues, which belongs to another Weyl chamber with the opposite ordering of the spectrum (see Fig. 2 for $N=2$ and 3).

Let us analyze the simplest case $N=2$, for which the simplex of eigenvalues is equivalent to an interval [0,1], while the intervals $[0,1/2)$ and $(1/2,1]$ form two Weyl chambers. A unitary orbit generated by each point of a Weyl chamber has the structure of the sphere S^2. The above statement has an intuitive interpretation: the minimal distance between two concentric spheres is equal to the distance between two of their points belonging to the same radius of the ball. The maximal distance between these spheres equals the distance between their points placed at the diameter of the ball on the other sides of its center. For example, consider two states in the Bloch ball. The radius of a given state is determined by its entropy, which in this case completely determines the entire spectrum. Hence two unitary orbits form two concentric spheres of different radii. Common eigenbases correspond to a common axis; hence the closest and furthest states both lie on the same axis, either both on the same side or on opposite sides of the center, respectively.

The above property shows that, in looking for a set of perfectly distinguishable states in a certain set R of mixed states that is invariant with respect to the unitary rotations, it is enough to analyze the subset of diagonal matrices.

Proposition 3. Let R_Δ be an arbitrary convex subset of the $(N-1)$-dimensional simplex of the eigenvalues. Let R denote the set of quantum states obtained from this set by any unitary rotation $R:=\{\rho\in\mathcal{M}_N:\rho=U[\mathrm{diag}(p)]U^\dagger$, and $p\in R_\Delta\}$. Let $k\leq N$ be a number such that $\Delta_{k-1}\in R_\Delta$ and there exists no $\Delta_k\in R_\Delta$. Then the maximal number of perfectly distinguishable states in R is equal to k, so it is equal to the maximal number of diagonal distinguishable states.

As before, the symbol Δ_k represents a regular k-dimensional simplex containing $k+1$ points separated by the maximal distance $D^{\max}$ with respect to the trace (or Bures) distance. Let us emphasize again that the geometry induced by the Bures metric differs considerably with respect to the flat Euclidean geometry induced by the HS metric. For instance, the simplex of eigenvalues for $N=3$ forms a flat equilateral triangle (of side $\sqrt{2}$) in the HS case, while it is equivalent to the octant of a sphere S^2 for the Bures distance.

V. CONCLUSIONS

In this work we commenced with the analysis of the geometry of the problem of quantum distinguishability. We showed that the problem of finding the maximal number of perfectly distinguishable states in a certain set R containing quantum states is equivalent to finding the dimension of the largest simplex of a fixed side size which can be embedded inside the set R. For this purpose one cannot use Euclidean simplices defined by the HS distance, but must use simplices with respect to Bures or trace distances.

The fidelity between any two quantum states is shown to be bounded by the classical fidelities between both spectra put in the same order (upper bound) or in the opposite order (lower bound). This observation implies that bounds for the Bures distance between two quantum states are achieved for diagonal states. Thus, in looking for distinguishable states in a rotationally invariant subset of the set of quantum states it is sufficient to restrict analysis to a smaller set of classical states, which correspond to diagonal density matrices.

Phrasing problems in geometric terms can be useful in developing intuition, often leading to connections to other

problems, and even helping with calculations. Although we have only started in the development of this approach here, we hope that these foundations and techniques will prove useful in the future for quantum state discrimination.

Note added in proof. Recently, we have learned that our Theorem IV follows from certain consequences of the theorem of Lidskii presented in chapters III.4 and IV.3 of the book of Bhatia [27]. We are grateful to J. Eisert for this remark.

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APPENDIX A: BOUND FOR THE TRACE OF A PRODUCT OF STATES

Let $\rho=\rho^\dagger$ and $\sigma=\sigma^\dagger$ denote two Hermitian operators acting on an N-dimensional Hilbert space. As throughout the paper, their spectra will be denoted by $p=\mathrm{eig}(\rho)$ and $q=\mathrm{eig}(\sigma)$, respectively. Let $p^\downarrow$ and $q^\downarrow$ denote the N-element vector of eigenvalues ordered in decreasing order, while the same spectra ordered increasingly will be written as $p^\uparrow$ and $q^\uparrow$. The symbol $(p^\uparrow)^s$ denotes the vector consisting of ordered elements of $p^\uparrow$, each component raised to power s.

Lemma 3. Let $\rho\geq 0$ and $\sigma\geq 0$ and let s,t denote positive real numbers. Then

$$(p^s)^\uparrow\cdot(q^t)^\downarrow \leq \mathrm{Tr}\,\rho^s\sigma^t \leq (p^s)^\uparrow\cdot(q^t)^\uparrow. \tag{A1}$$

Proof. Let $|\mu_i\rangle$ and $|\nu_j\rangle$ denote the eigenvectors of the states ρ and σ. We will start by finding a form of $\mathrm{Tr}\,\rho^s\sigma^t$, in terms of overlaps with a doubly stochastic matrix,

$$\mathrm{Tr}\,\rho^s\sigma^t = \mathrm{Tr}\left(\sum_{i,j} p_i^s q_j^t |\mu_i\rangle\langle\mu_i|\nu_j\rangle\langle\nu_j|\right) \tag{A2}$$

$$=\sum_{i,j} p_i^s q_j^t |\langle\mu_i|U|\mu_j\rangle|^2 \tag{A3}$$

$$=\sum_{i,j} p_i^s q_j^t B_{i,j}, \tag{A4}$$

where U is the unitary relating the two eigenbases $U|\mu_i\rangle=|\nu_i\rangle\ \forall\ i$ and $B:=\Sigma_{i,j}|U_{i,j}|^2|\mu_i\rangle\langle\mu_j|$ so that $B_{ij}=|U_{ij}|^2$. Hence the matrix B is by construction unistochastic [28] and thus bistochastic.

It is convenient to introduce here two non-normalized vectors $|\psi\rangle:=\Sigma p_i'|\mu_i\rangle$, and $|\phi\rangle:=\Sigma q_j'|\mu_j\rangle$, where $p_i'=p_i^s$ and $q_j'=q_j^t$ are non-negative. Then the trace can be rewritten in the form

$$\mathrm{Tr}\,\rho^s\sigma^t = \langle\psi|B|\phi\rangle. \tag{A5}$$

Birkhoff's theorem [25] states that any doubly stochastic matrix can be written as a finite convex combination of permutation matrices O_i; hence we write $B=\Sigma_i r_i O_i$, $\Sigma_i r_i=1$. Thus the extremum of a linear function of the bistochastic matrix B will be realized at one of its extremal points. There are exactly $N!$ of them, and among all possible permutations O_i the maximum is obtained if the orders of elements of both vectors are the same, while the minimum is achieved if the two spectra are in opposite order,

$$\langle\psi|B|\phi\rangle = \sum_i r_i\langle\psi|O_i|\phi\rangle \geq \langle\psi|O_{\min}|\phi\rangle = (p^\uparrow)^s\cdot(q^\downarrow)^t \tag{A6}$$

$$\leq \langle\psi|O_{\max}|\phi\rangle = (p^\uparrow)^s\cdot(q^\uparrow)^t. \tag{A7}$$

Since all components of the vector p (and q) are non-negative, raising each element to a positive exponent s (or t) will not change the order of the vector $(p^\uparrow)^s=(p^s)^\uparrow$. Putting it all together we arrive at (A1) and complete the proof. ■

For concreteness let us write down explicitly some special cases. In the simplest case $s=t=1$ one obtains

$$p^\uparrow\cdot q^\downarrow \leq \mathrm{Tr}\,\rho\sigma \leq p^\uparrow\cdot q^\uparrow, \tag{A8}$$

while on setting $s=t=1/2$ one obtains inequality (4.7) used in the proof of inequality (4.9).

An analog of Lemma 2 may be obtained in the case where one of the two operators is not positive.

Lemma 4. Consider a positive number $s>0$, a state $\rho\geq 0$, and a Hermitian operator $\sigma=\sigma^\dagger$ not necessarily positive. Then

$$(p^s)^\uparrow\cdot q^\downarrow \leq \mathrm{Tr}\,\rho^s\sigma \leq (p^s)^\uparrow\cdot q^\uparrow. \tag{A9}$$

Proof of this lemma is similar to the proof of Lemma 2. In this case the vector q of eigenvalues of operator σ contains in general also negative entries, so the vector $|\phi\rangle:=\Sigma_j q_j|\mu_j\rangle$ is given by a pseudomixture with some weights negative. Constructing unitary bases U and the bistochastic matrix M, one may write the analyzed trace in the form (A5) and make use of the Birkhoff theorem. Since the operator ρ with spectrum p is positive, raising its components to a positive power will not change the order, $(p^\uparrow)^s=(p^s)^\uparrow$. Therefore we may perform the last step analogous to (A7), obtaining the desired result. ■

APPENDIX B: BOUND FOR THE TRACE OF A DIFFERENCE OF TWO STATES

In this appendix we prove the following lemma.

Lemma 5. Let A and B denote Hermitian matrices of size n. Let us order their eigenvalues in decreasing order, $\lambda_1(A)\geq\cdots\geq\lambda_n(A)$ and $\lambda_1(B)\geq\cdots\geq\lambda_n(B)$. Then the following upper bound for the trace of the absolute value of the difference holds:

$$\mathrm{Tr}|A-B| = \sum_{i=1}^n \sigma_i(A-B) \leq \sum_{i=1}^n |\lambda_i(A)-\lambda_{n+1-i}(B)|. \tag{B1}$$

Proof. Let us express both operators in their eigenrepresentation $A=\Sigma_i^n p_i|\mu_i\rangle\langle\mu_i|$ and $B=\Sigma_i^n q_i|\nu_i\rangle\langle\nu_i|$, where for convenience we have introduced the notation $p_i=\lambda_i(A)$ and

$q_i=\lambda_i(B)$. Making use of Eq. (4.11) and basic properties of the trace, we get

$$\mathrm{Tr}|A-B| = \max_U |\mathrm{Tr}\, AU - \mathrm{Tr}\, BU| \tag{B2}$$

$$= \max_U \left| \sum_{i=1}^n p_i \langle \mu_i|U|\mu_i\rangle - q_i\langle \nu_i|U|\nu_i\rangle \right|. \tag{B3}$$

Since $|\langle \mu_i|U|\mu_i\rangle| \le 1$, $|\langle \nu_i|U|\nu_i\rangle| \le 1$, and $\mathrm{Tr}\, U = \sum_{i=1}^n \langle \mu_i|U|\mu_i\rangle = \sum_{i=1}^n \langle \nu_i|U|\nu_i\rangle$, we have

$$\mathrm{Tr}|A-B| \le \max\left\{ \left| \sum_{i=1}^n \xi_i p_i - \zeta_i q_i \right| : |\xi_i| \le 1, |\zeta_i| \le 1 \right.$$
$$\left. \text{for } i=1,\ldots,n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\}. \tag{B4}$$

For fixed values of ξ_i and ζ_i we denote $s=\sum_{i=1}^n \xi_i p_i - \zeta_i q_i$. Let $s=ce^{i\varphi}$; we have

$$c = |s| = \left| \frac{s}{e^{i\varphi}} \right| = \left| \sum_{i=1}^n \frac{\xi_i}{e^{i\varphi}} p_i - \frac{\zeta_i}{e^{i\varphi}} q_i \right|.$$

Because $|\frac{\xi_i}{e^{i\varphi}}| \le 1$ and $|\frac{\zeta_i}{e^{i\varphi}}| \le 1$, we can without loss of generality assume that $s \in \mathbb{R}$. Note now that under this assumption we have

$$\max\left\{ \left| \sum_{i=1}^n \xi_i p_i - \zeta_i q_i \right| : |\xi_i| \le 1, |\zeta_i| \le 1 \right.$$
$$\left. \text{for } i=1,\ldots,n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i, \right\} \tag{B5}$$

$$= \max\left\{ \left| \sum_{i=1}^n \mathrm{Re}(\xi_i) p_i - \mathrm{Re}(\zeta_i) q_i \right| : |\xi_i| \le 1, |\zeta_i| \le 1 \right.$$
$$\left. \text{for } i=1,\ldots,n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i, \right\} \tag{B6}$$

$$= \max\left\{ \left| \sum_{i=1}^n \xi_i p_i - \zeta_i q_i \right| : -1 \le \xi_i \le 1, -1 \le \zeta_i \le 1 \right.$$
$$\left. \text{for } i=1,\ldots,n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i, \right\}. \tag{B7}$$

The term $\sum_{i=1}^n \xi_i p_i - \zeta_i q_i$ is a linear function of $2n$ variables $\xi_1,\ldots,\xi_n$, $\zeta_1,\ldots,\zeta_n$, so it reaches its extreme value at the edges of the polygon defined by

$$\left\{ -1 \le \xi_i \le 1, \quad -1 \le \zeta_i \le 1 \right.$$
$$\left. \text{for } i=1,\ldots,n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\}. \tag{B8}$$

Thus we can focus on the edges of the polygon

$$\left\{ \xi_i \in \{-1,1\}, \quad \zeta_i \in \{-1,1\} \right.$$
$$\left. \text{for } i=1,\ldots,n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\}. \tag{B9}$$

Note that we obtain the maximum if in the sum $\sum_{i=1}^n \xi_i p_i + (-\zeta_i) q_i$ the n maximum values of $\{p_1,\ldots,p_n,q_1,\ldots,q_n\}$ will be equipped with coefficient $+1$ and n minimum values with -1. Because $p_1 \ge p_2 \ge \cdots \ge p_n$ and $q_1 \ge q_2 \ge \cdots \ge q_n$, we can thus write the n maximum values as

$$\max\{p_1,q_n\}, \max\{p_2,q_{n-1}\}, \ldots, \max\{p_n,q_1\}, \tag{B10}$$

and the n minimum values as

$$\min\{p_1,q_n\}, \min\{p_2,q_{n-1}\}, \ldots, \min\{p_n,q_1\}. \tag{B11}$$

So the maximum value of

$$\max\left\{ \left| \sum_{i=1}^n \xi_i p_i - \zeta_i q_i \right| : \xi_i \in \{-1,1\}, \quad \zeta_i \in \{-1,1\} \right.$$
$$\left. \text{for } i=1,\ldots,n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\} \tag{B12}$$

is equal to

$$\left| \sum_{i=1}^n \max\{p_i,q_{n-i+1}\} - \min\{p_i,q_{n-i+1}\} \right| = \sum_{i=1}^n |p_i - q_{n-i+1}|. \tag{B13}$$

This gives us the required upper bound (B1). ■

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